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Stochastic Time-Dependent Current-Density Functional Theory[1]

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Static and dynamical density functional methods have been applied with a certain degree of success to a variety of closed quantum mechanical systems, i.e., systems that can be described via a Hamiltonian dynamics. However, the relevance of open quantum systems - those coupled to external environments, e.g., baths or reservoirs - cannot be overestimated. To investigate open quantum systems with DFT methods we have introduced a new theory, we have named Stochastic Time-Dependent Current Density Functional theory (S-TDCDFT) [1]: starting from a suitable description of the system dynamics via a *stochastic* Schrödinger equation [2], we have proven that given an initial quantum state and the coupling between the system and the environment, there is a one-to-one correspondence between the ensemble-averaged current density and the external vector potential applied to the system.

In this talk, I will introduce the stochastic formalism needed for the description of open quantum systems, discuss in details the theorem of Stochastic TD-CDFT, and provide few examples of its applicability like the dissipative dynamics of excited systems, quantum-measurement theory and other applications relevant to charge and energy transport in nanoscale systems.

[1] M. Di Ventra and R. D'Agosta, Physical Review Letters **98**, 226403 (2007)

[2] N.G. van Kampen, *Stochastic processes in Physics and Chemistry*, (North Holland, 2001), 2nd ed.

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